

Quantum mechanical picture of the coupling between interlayer electronic excitations and infrared active phonons in bilayer cuprate superconductors

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(Dated: March 1, 2013)

The formula frequently used to describe the c -axis infrared response of the coupled electron-phonon system of bilayer cuprate superconductors and providing important insights into the physics of these materials has been originally obtained at the level of the phenomenological multilayer model. Here we derive it using diagrammatic perturbation theory.

PACS numbers: 74.25.Gz, 74.72.-h

The phase diagram of underdoped high- T_c cuprate superconductors is divided into three regions: the superconducting one below T_c , the pseudogap phase in the temperature range $T_c < T < T^*$, where T^* is the onset temperature of the (high energy) pseudogap, and the anomalous normal state above T^* .^{1,2} There is an interesting and important class of physical properties, that begin to develop/whose temperature dependence changes its character at an onset temperature much lower than T^* but at the same time considerably higher than T_c .³ These include, e.g., the NMR relaxation rate ($1/T_1T$),⁴ amplitude of the transverse plasma mode (also referred to as the 400 cm^{-1} mode) and some phonon structures in the c -axis infrared conductivity of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (Y-123)⁵⁻¹⁰, in-plane scattering rate and in-plane conductivity below ca 700 cm^{-1} ,^{3,10} amplitude of the neutron resonance¹¹, Nernst signal¹², diamagnetic response¹³, specific heat¹⁴, some features of the excitation gap^{15,16}, spectral weight at the chemical potential¹⁷, magnetic field dependence of the in-plane resistivity¹⁸, THz conductivity^{19,20}, and the quasiparticle interference²¹. The values of the onset temperature range from ca 15 K above T_c (THz conductivity) to more than 100 K above T_c (transverse plasmon and the phonon structures, Nernst). Some of the phenomena (increase of the THz conductivity and quasiparticle interference) are almost certainly related to superconducting fluctuations. Some other with a much higher onset temperature (e.g., the transverse plasmon and the phonon structures, Nernst), have also been attributed to a precursor superconducting state (PSC) lacking the long range phase coherence. This exciting issue, however, is fairly controversial and no consensus has been reached thus far. There are two prerequisites for an ultimate understanding: (a) A detailed knowledge of both doping (p) and temperature dependence of the relevant quantities. (b) An understanding of the physical contents of these quantities, in particular, the relation to superconductivity.

Dubroka *et al.*¹⁰ have studied in detail the temperature dependence of the phonon structures in the infrared c -axis conductivity of Y-123 for a broad range of p of $0.03 < p < 0.17$ and determined the p -dependence of the corresponding onset temperature T^{ons} . The relation be-

tween the phonons and the electronic degrees of freedom has been understood in terms of the phenomenological, essentially classical, multilayer model^{22,23}, involving the local conductivity of the bilayer units (denoted here as σ_{bl}) and that of the spacing layers (σ_{int}), extended^{24,25} by including formulas for the local fields acting on the relevant ions and a feedback of the phonons. For a schematic representation of the electronic part of the model, see Fig. 1 (b) of Ref. 26. For a careful discussion of the role of the phonons, see Ref. 25. The model has allowed the authors of Ref. 10 to conclude that at T^{ons} the spectral weight of the low-energy component of σ_{bl} (the Drude peak in the analysis of Fig. 1 of Ref. 10) begins to increase, signalling an increase of coherence of the response. Several arguments have been advanced suggesting that this is due to the formation of a PSC. The importance of the topic of PSC and of other interesting fields of application of the multilayer model²⁷⁻³⁰ calls for developing a fully quantum mechanical description of the response of the coupled electron-phonon system, that would support the phenomenological approach. Chaloupka, Bernhard, and Munzar have already constructed (see Ref. 26, CBM in the following) a microscopic gauge-invariant theory of the c -axis infrared response of bilayer cuprate superconductors, such as Y-123, providing both a justification and limits of the electronic part of the multilayer model and of a related earlier approach³¹. The phonons, however, have not yet been incorporated. Here we provide an extension of the theory of CBM, where they are included at the Green's function level. A similar approach has been recently used to explain the electric field dependence of the infrared spectra of bilayer graphene³². The formula for the c -axis conductivity will be derived and it will be shown to coincide, for a natural choice of the electron-phonon coupling term, with that of the phenomenological model. The essential aspects of the theory are formulated in the points (i)-(viii).

For the sake of simplicity we neglect the hopping through the spacing layer (t'_\perp in the notation of CBM, $\sigma_{\text{int}} = 0$), focus, as usual, on the long-wavelength limit, $\mathbf{q} = 0$,³³ and limit ourselves to the case of one infrared active phonon.

(i) *Relevant equations of CBM.* The (electronic) con-

ductivity σ_{bl} of the bilayer unit is given by

$$\sigma_{bl}(\omega) = -i\omega\varepsilon_0\chi_{bl}(\omega) = \frac{\kappa_{dia-bl} + d_{bl}\Pi_{jj}(\omega)}{i(\omega + i\delta)}, \quad (1)$$

where χ_{bl} is the bilayer susceptibility, κ_{dia-bl} the term describing the diamagnetic contribution, d_{bl} the distance between the closely spaced planes, and $\Pi_{jj}(\omega)$ the current-current correlation function. The term κ_{dia-bl} is given by

$$\kappa_{dia-bl} = -\frac{e^2 d_{bl}}{\hbar^2 N a^2} \sum_{\mathbf{k}s} t_{\perp}(\mathbf{k}) \langle c_{B\mathbf{k}s}^{\dagger} c_{B\mathbf{k}s} - c_{A\mathbf{k}s}^{\dagger} c_{A\mathbf{k}s} \rangle, \quad (2)$$

where N is the number of surface unit cells per copper-oxygen plane, a is the in-plane lattice parameter, the sum runs over all values of the in-plane quasimomentum \mathbf{k} and spin s , $t_{\perp}(\mathbf{k})$ is the intra-bilayer hopping parameter, and $c_{B\mathbf{k}s}^{\dagger}$, $c_{B\mathbf{k}s}$ ($c_{A\mathbf{k}s}^{\dagger}$, $c_{A\mathbf{k}s}$) are the quasiparticle operators corresponding to the bonding (antibonding) band. The correlator Π_{jj} is given by

$$\Pi_{jj}(\omega) = \frac{iNa^2}{\hbar} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle [\hat{j}_{bl}^p(t), \hat{j}_{bl}^p(0)] \rangle \theta(t), \quad (3)$$

where \hat{j}_{bl}^p is the operator of the intrabilayer paramagnetic current density,

$$\hat{j}_{bl}^p = \frac{ie}{\hbar Na^2} \sum_{\mathbf{k}s} t_{\perp}(\mathbf{k}) \left(c_{B\mathbf{k}s}^{\dagger} c_{A\mathbf{k}s} - c_{A\mathbf{k}s}^{\dagger} c_{B\mathbf{k}s} \right). \quad (4)$$

In the absence of interlayer Coulomb interaction and any phonon contribution, the total (volume averaged) c -axis current density would be equal to $\sigma^*(\omega)E^{\text{ext}}(\omega)$ with $\sigma^*(\omega) = (d_{bl}/d)\sigma_{bl}(\omega)$ and E^{ext} the external field, d is the c -axis lattice parameter.

(ii) *Response of a c -axis polarized infrared active phonon mode.* In the absence of any electronic contribution, the current density can be expressed as $\sigma^*(\omega)E^{\text{ext}}(\omega)$ with

$$\sigma^*(\omega) = \sigma_{ph}(\omega) = -i\omega\varepsilon_0\chi = \frac{\kappa_{dia-ph} + d\Lambda_{jj}(\omega)}{i(\omega + i\delta)}, \quad (5)$$

where χ is the phonon polarizability, κ_{dia-ph} the term describing the diamagnetic contribution, and $\Lambda_{jj}(\omega)$ the phonon current-current correlator. The term κ_{dia-ph} is equal to $-\varepsilon_0\omega_P^2$, where ω_P is the phonon plasma frequency, $\omega_P^2 = 1/(a^2 d \varepsilon_0) \left(\sum_{\mu} [e_{\mu}(\mathbf{e})_{\mu z} / \sqrt{m_{\mu}}] \right)^2$. Here e_{μ} , $(\mathbf{e})_{\mu z}$ and m_{μ} are the effective charge, the c -axis component of the polarization vector and the mass of the μ -th ion. The correlator is given by

$$\Lambda_{jj}(\omega) = \frac{iNa^2}{\hbar} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle [\hat{j}_{ph}^p(t), \hat{j}_{ph}^p(0)] \rangle \theta(t). \quad (6)$$

Here \hat{j}_{ph}^p is the phonon paramagnetic current-density operator,

$$\hat{j}_{ph}^p = \frac{i}{a^2 d} \sqrt{\frac{\hbar\omega_0}{2}} \sum_{\mu} \frac{e_{\mu}(\mathbf{e})_{\mu z}}{\sqrt{m_{\mu}}} (a^{\dagger} - a), \quad (7)$$

ω_0 the phonon frequency, a^{\dagger} and a are the phonon creation and annihilation operators, respectively. The correlator can be further expressed in terms of the retarded phonon propagator $D(\omega)$:

$$d\Lambda_{jj} = \varepsilon_0\omega_0^2\chi = -\frac{\varepsilon_0\omega_P^2\omega_0}{2}D(\omega). \quad (8)$$

In the noninteracting case,

$$D(\omega) = D_0(\omega) = 2\omega_0/(\omega^2 - \omega_0^2 + i\omega\delta).$$

(iii) *Case of the electronic contribution coexisting with the phonon one.* The total current density is given by $\sigma^*(\omega)E^{\text{ext}}$ with

$$\sigma^*(\omega) = \frac{\kappa'_{dia-bl} + \kappa_{dia-ph} + d\Xi_{jj}(\omega)}{i(\omega + i\delta)}, \quad (9)$$

where $\kappa'_{dia-bl} = (d_{bl}/d)\kappa_{dia-bl}$,

$$\Xi_{jj}(\omega) = \frac{iNa^2}{\hbar} \int_{-\infty}^{\infty} dt e^{i\omega t} \times \\ \times \langle [\hat{j}_{bl}^p(t) + \hat{j}_{ph}^p(t), \hat{j}_{bl}^p(0) + \hat{j}_{ph}^p(0)] \rangle \theta(t) \quad (10)$$

and $\hat{j}_{bl}^p = (d_{bl}/d)\hat{j}_{bl}^p$. In the absence of interlayer Coulomb interaction and electron-phonon interaction, the mixed correlators (involving both \hat{j}_{bl}^p and \hat{j}_{ph}^p) would vanish and we would obtain simply $\sigma^*(\omega) = (d_{bl}/d)\sigma_{bl}(\omega) + \sigma_{ph}(\omega)$ with σ_{bl} from Eq. (1) and σ_{ph} from Eq. (5). The interactions will be shown to lead both to a renormalization of σ_{bl} and σ_{ph} and to nonzero values of the mixed correlators.

(iv) *Formulas used to describe the final state interactions.* Let us begin our considerations with the simple scheme of Fig. 1 (b) of CBM. The difference between the local conductivities σ_{bl} and σ_{int} leads to a difference between the current densities j_{bl} and j_{int} resulting in a charge redistribution between the CuO_2 planes, that can be characterized by the excess surface charge density ρ of the bottom plane (the density of the upper plane is $-\rho$). The electrostatic energy due to ρ is given by $Na^2 d_{bl} \rho^2 / (2\varepsilon_0)$ and the corresponding contribution to the Hamiltonian by Eq. (25) of CBM, i.e.,

$$H_C = \frac{Na^2 d_{bl}}{2\varepsilon_0} \hat{\rho}^2, \quad (11)$$

where $\hat{\rho}$ is the density operator, that can be expressed in terms of the quasiparticle operators as

$$\hat{\rho} = \frac{e}{2Na^2} \sum_{\mathbf{k}s} \left(c_{A\mathbf{k}s}^{\dagger} c_{B\mathbf{k}s} + c_{B\mathbf{k}s}^{\dagger} c_{A\mathbf{k}s} \right). \quad (12)$$

Next we derive the formula for the coupling term H_{e-p} describing the interaction between the surface charge densities of the planes ρ and $-\rho$ and a phonon. We begin with the textbook formula for the energy U of a polarized medium in a homogeneous electric field: $U = -V \cdot P \cdot E$,

where V is the volume of the medium, P the polarization and E the field. In the present case, V is the volume of N unit cells, $V \rightarrow Na^2d$, P is the polarization due to the phonon, $P \rightarrow \hat{P}$,

$$\hat{P} = \frac{1}{a^2d} \sqrt{\frac{\hbar}{2\omega_0}} \sum_{\mu} \frac{e_{\mu}(\mathbf{e})_{\mu z}}{\sqrt{m_{\mu}}} (a^{\dagger} + a), \quad (13)$$

and E is the electric field due to ρ and $-\rho$, $E \rightarrow \hat{\rho}/\varepsilon_0$. In addition, the product has to be multiplied by a factor denoted by ξ , representing the degree of overlap of E and the microscopic dipoles (E is nonzero only in the bilayer unit); $\xi = 1(0)$ for phonons associated with vibrations inside the bilayer unit (outside the bilayer unit) and $\xi \approx 1/2$ for phonons involving mainly the oxygens of the CuO_2 planes. By combining the expressions for V , P , and E we obtain

$$H_{e-p} = -\xi \frac{Na^2d}{\varepsilon_0} \hat{P} \hat{\rho}. \quad (14)$$

(v) *Modification of the response by H_C and H_{e-p} .* The function Ξ_{jj} defined by Eq. (10) can be written as the sum of four contributions: χ_A [the term involving $\hat{J}_{bl}^p(t)$ and $\hat{J}_{bl}^p(0)$], χ_B [$\hat{J}_{ph}^p(t)$ and $\hat{J}_{ph}^p(0)$], χ_C [$\hat{J}_{bl}^p(t)$ and $\hat{J}_{ph}^p(0)$], and χ_D [$\hat{J}_{ph}^p(t)$ and $\hat{J}_{bl}^p(0)$]. These correlators can be expressed, using perturbation theory, in terms of those referring to the case of $H_C = 0$ and $H_{e-p} = 0$: Π_{jj} , $\Pi_{j\rho}$, $\Pi_{\rho j}$, $\Pi_{\rho\rho}$, Λ_{jj} , Λ_{jP} , Λ_{Pj} and Λ_{PP} . Two of the latter, Π_{jj} and Λ_{jj} , have been defined above, see Eqs. (3) and (6), the others are defined similarly, for example $\Lambda_{jP}(\omega) = (iNa^2/\hbar) \int_{-\infty}^{\infty} dt e^{i\omega t} \langle [\hat{J}_{ph}^p(t), \hat{P}(0)] \rangle \theta(t)$. Figure 1 shows the Feynman diagrams representing the correlators [in a) and b)] and the interaction vertices [in c)]. Also shown are the factors to be assigned to the vertices when calculating the contributions of the diagrams. Figure 2 shows the series of the diagrams corresponding to χ_A , χ_C , χ_C and χ_D . The series can be summed up by standard techniques³⁴ and the results are

$$\begin{aligned} \left(\frac{d}{d_{bl}}\right)^2 \chi_A &= \Pi_{jj} + \Pi_{j\rho} \frac{1}{1 - \Pi'_{\rho\rho}} \Pi'_{\rho j}, \\ \chi_B &= \Lambda_{jj} + \frac{\xi^2 d^2}{\varepsilon_0^2} \Lambda_{jP} \frac{\Pi_{\rho\rho}}{1 - \Pi'_{\rho\rho}} \Lambda_{Pj}, \\ \frac{d}{d_{bl}} \chi_C &= \frac{\xi d}{\varepsilon_0} \Pi_{j\rho} \frac{1}{1 - \Pi'_{\rho\rho}} \Lambda_{Pj}, \\ \frac{d}{d_{bl}} \chi_D &= \frac{\xi d}{\varepsilon_0} \Lambda_{jP} \frac{1}{1 - \Pi'_{\rho\rho}} \Pi_{\rho j}, \end{aligned} \quad (15)$$

where $\Pi'_{\rho\rho/\rho j}$ is the expression corresponding to the repeating segment of the diagrams shown in Fig. 1 (d),

$$\Pi'_{\rho\rho/\rho j} = \frac{d_{bl}}{\varepsilon_0} \left(\frac{\xi^2 d^2}{d_{bl} \varepsilon_0} \Lambda_{PP} - 1 \right) \Pi_{\rho\rho/\rho j}. \quad (16)$$

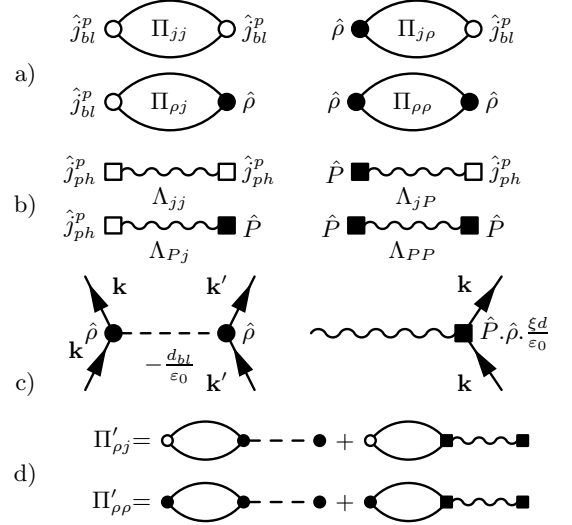


FIG. 1: Feynman diagrams representing the correlators defined in the text [a) and b)], the interaction vertices corresponding to H_C of Eq. (11) and H_{e-p} of Eq. (14) [c)], and two segments that appear in the series shown in Fig. 2 [d)].

(vi) *Simplifications resulting from the gauge invariance.* The sum in the numerator on the right hand side of Eq. (9) containing $\kappa_{\text{dia-bl}}$, $\kappa_{\text{dia-ph}}$ and the four correlators of Eq. (15) can be considerably simplified by using the relations:

$$\begin{aligned} \Pi_{\rho j} &= \frac{i\omega\varepsilon_0}{d_{bl}} \chi_{bl} = -\Pi_{j\rho}, \quad \Pi_{\rho\rho} = \frac{\varepsilon_0}{d_{bl}} \chi_{bl}, \\ \Lambda_{Pj} &= \frac{i\omega\varepsilon_0}{d} \chi = -\Lambda_{jP}, \quad \Lambda_{PP} = \frac{\varepsilon_0}{d} \chi, \end{aligned} \quad (17)$$

that follow from the requirement of the charge conservation formulated in different gauges of the electromagnetic potentials or equivalently from the requirement of the gauge invariance^{26,35}. We obtain

$$\sigma^*(\omega) = -i\omega\varepsilon_0 \frac{(d_{bl}/d)\chi_{bl} + \chi + (1 - 2\xi)\chi_{bl}\chi}{1 - \chi_{bl}[(d/d_{bl})\xi^2\chi - 1]}. \quad (18)$$

(vii) *Total electric field, from $\sigma^*(\omega)$ to $\sigma(\omega)$.* The total electric field E consists of the external field E^{ext} and the induced field E^{ind} due to the charge fluctuations described by ρ and the phonon polarization described by P , $E^{\text{ind}} = (d_{bl}/d)(\rho/\varepsilon_0) - (P/\varepsilon_0) = j/(i\omega\varepsilon_0)$. We have used the continuity equation, $i\omega\rho = j_{bl}$ and the relation between P and the total phonon current density j_p , $-i\omega P = j_p$, j is the total current density. The c -axis conductivity $\sigma(\omega)$ defined by $\sigma(\omega) = j(\omega)/E(\omega)$ is equal to $\sigma^*(\omega)[E^{\text{ext}}(\omega)/E(\omega)]$, i.e.,

$$\begin{aligned} \sigma(\omega) &= \frac{\sigma^*(\omega)}{1 - i\sigma^*/(\omega\varepsilon_0)} = \\ &= -i\omega\varepsilon_0 \frac{(d_{bl}/d)\chi_{bl} + \chi + (1 - 2\xi)\chi_{bl}\chi}{1 + [1 - (d_{bl}/d)]\chi_{bl} - \chi - [1 - 2\xi + (d_{bl}/d)\xi^2]\chi_{bl}\chi}. \end{aligned} \quad (19)$$

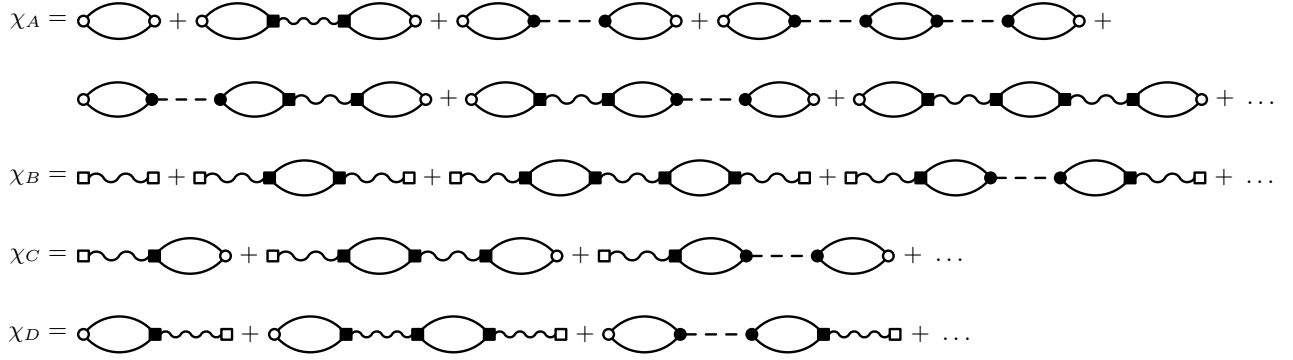


FIG. 2: Series of the diagrams corresponding to the quantities χ_A , χ_B , χ_C , and χ_D defined in the text. The sum of the contributions of the diagrams is to be multiplied by d_{bl}^2/d^2 in case of χ_A and by d_{bl}/d in case of χ_C and χ_D .

(viii) Considerations of *screening by high frequency processes* lead to a slightly modified formula:

$$\sigma(\omega) = \text{r. h. s. of (19)} \left[\varepsilon_0 \rightarrow \varepsilon_0 \varepsilon_\infty, \chi_{\text{bl}} \rightarrow \frac{\chi_{\text{bl}}}{\varepsilon_\infty}, \chi \rightarrow \frac{\chi}{\varepsilon_\infty} \right], \quad (20)$$

where ε_∞ is the interband dielectric function. The total dielectric function is given by $\varepsilon(\omega) = \varepsilon_\infty + i\sigma(\omega)/(\omega\varepsilon_0)$.

It is an easy exercise to show that the final formula [(19) or (20)] is precisely the same as the one resulting from the single phonon version of the phenomenological multilayer model.³⁶ The important point is that it has been derived here on microscopic grounds, using perturbation theory, with the electron-phonon coupling constant determined by simple electrostatics. Within the phenomenological model, the response of a phonon to the applied field is governed by the eigenvector-dependent local electric field. Here, the eigenvector enters the equations through the coupling constant. Our result adds

credibility to the central claim of Ref. 10, that at T_{ons} the spectral weight of the low-energy component of the (local) intralayer conductivity σ_{bl} begins to increase, possibly a manifestation of precursor superconductivity. Future studies involving the present formalism in conjunction with the local conductivities resulting from microscopic calculations such as those reported in CBM (rooted in the Fermi liquid theory) or those of the kind of Ref. 37 based on a phenomenological ansatz³⁸ related to the resonating valence bond picture are needed to achieve a further progress.

This work was supported by the Ministry of Education of Czech Republic (MSM0021622410), by the project CEITEC - Central European Institute of Technology (CZ.1.05/1.1.00/02.0068) from European Regional Development Fund and by the internal project MUNI/A/1047/2009. We gratefully acknowledge discussions with J. Chaloupka and A. Dubroka.

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